ISOTOPIC SUBSTITUTIONS UNVEILED THE IDENTIFICATION OF THE MORE STABLE CONFORMER OF FENCHOL AND OF ITS WATER COMPLEX

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Fenchol $C_{10}H_{18}O$ was identified as one of the many products emitted by several plants, by pin radiata wood, and by fibers panels [a]. It is a monoterpene of spectroscopic interest in order to determine the more stable conformer. Indeed the fenchol molecule presents two stereoisomers depending on the position of the OH group and of the hydrogen atom, named endo- and exo-fenchol.

In the present work, we present the conformational landscape study of fenchol in order to identify in the gas phase the more stable conformer for each stereoisomer. A combination of theoretical calculations and Fourier transform microwave spectroscopy in a supersonic molecular jet was used. Because of a disagreement between the different calculation methods for the endo-fenchol stereoisomer, fenchol-D was used to identify the most stable conformer. The hyperfine structure signature was found very helpful.

Moreover the hydration of endo-fenchol was studied. The multi-isotopic substitution of deuterium has led to identify the observed conformer. Surprisingly the substituted structure of the hydrogen atoms shows that the observed complex is formed by hydrogen bonding between the high energy conformer of endo-fenchol - which is not observed in the jet - with the water molecule. The set of molecular parameters was adjusted using a Watson Hamiltonian in the A reduction to the experimental accuracy.

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